The discrete Moser–Veselov algorithm for the free rigid body

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Overview

The subject of this talk is the numerical solution of the free RB equations,

$$M' = [M, \Omega], \qquad M = \Omega J + J\Omega,$$

where M, Ω are skew-symmetric matrices and J is a diagonal matrix with positive entries.

M is the matrix of **body momenta**

Ω is the matrix of **body angular velocity**

Often the above equations are associated with the equations that give the configuration of the body in the fixed frame,

$$Q' = Q\Omega, \qquad Q \in \mathrm{SO}(N).$$

- The Discrete Moser–Veselov description of the rigid body
- Integrability of the discrete algorithm
- Backward error analysis of the the DMV algorithm
- Higher order integrable approximations
- Numerical experiments and comparisons with other methods
- Explicit methods for the 3×3 case

The Moser–Veselov discrete version of the dynamics of a Rigid Body

The Lagrangian of the continuous RB equations, is the kinetic energy,

$$L = \frac{1}{2}\mathrm{tr}(\Omega^\top M) = \frac{1}{2}\mathrm{tr}(-\Omega^2 J - \Omega J \Omega) = \mathrm{tr}(\Omega^\top J \Omega), \tag{1}$$

where we take into account that $\Omega^\top = -\Omega$ and that the trace is invariant under cyclic permutations. Following (Marsden, Pekarsky & Shkoller 1999), discretise $\Omega = X^{-1}\dot{X}$, where $X \in \mathrm{SO}(N)$ is the configuration of the body, using a finite difference approximation of the derivative,

$$\Omega = X^{-1}\dot{X} \approx \frac{1}{h} X_{k+1}^\top (X_{k+1} - X_k), \qquad X_k, X_{k+1} \in \mathrm{SO}(N),$$

which gives

$$L \approx \frac{1}{h^2}\mathrm{tr}(J - X_k^\top X_{k+1} J - J X_{k+1}^\top X_k - X_k^\top X_{k+1} J X_{k+1}^\top X_k).$$

Due to the orthogonality of the X_k's and the cyclicity of the trace, the first and the last term cancel, and moreover, we can write

$$L \approx \frac{2}{h^2}\mathrm{tr}(X_k J X_{k+1}^\top).$$

Up a scaling factor, this is precisely the discrete Lagrangian of Moser and Veselov.

Consider the fuctional $S(X)$ determined by

$$S = \sum_k \mathrm{tr}(X_k J X_{k+1}^\top)$$

where $X = \{X_k\}$ with $X_k \in \mathrm{O}(N)$ and J is a diagonal matrix. To obtain the stationary points of S, we consider

$$\sum_k \mathrm{tr}(X_k J X_{k+1}^\top) - \frac{1}{2} \sum_k \mathrm{tr}(\Lambda_k (X_k X_k^\top - I)),$$

(where $\Lambda_k = \Lambda_k^\top$ is a Lagrange multiplier), and $\delta S = 0$ becomes

$$X_{k+1} J + X_{k-1} J = \Lambda_k X_k,$$

from which, multiplying by $X_k^\top$ on the right and taking into consideration the symmetry of Λ_k,

$$X_{k+1} J X_k^\top + X_{k-1} J X_k^\top = \Lambda_k = \Lambda_k^\top = X_k J X_{k+1}^\top + X_k J X_{k-1}^\top, \tag{2}$$

hence, the *discrete analogue of the angular momentum in space*,

$$m_k = X_k J X_{k-1}^\top - X_{k-1} J X_k^\top,$$

is conserved.

In the body variables, setting $\omega_k = X_k^\top X_{k-1} \in \mathrm{O}(N)$ and $M_k = X_{k-1}^{-1} m_k X_{k-1} = \omega_k^\top J - J\omega_k \in \mathfrak{so}(N)^*$ (angular momentum w.r.t. the body), (2) becomes

$$\begin{aligned} M_{k+1} &= \omega_k M_k \omega_k^\top \\ M_k &= \omega_k^\top J - J\omega_k. \end{aligned} \tag{3}$$

the **discrete Euler–Arnold** equation.

In the continuous limit: when $t_k = t_0 + k\varepsilon$, $k = 0, 1, 2, \ldots$,

- $X_k = X(t_k)$
- $\omega_k = X_k^\top X_{k-1} \approx I - \varepsilon\Omega(t_k)$,
- $M_k \approx \varepsilon(J\Omega + \Omega J) = \varepsilon M(t_k)$,

letting $\varepsilon \to 0$, one obtains the familiar Euler–Arnold equations for the motions of the N-dimensional rigid body,

$$\begin{aligned} M' &= [M, \Omega] \\ M &= J\Omega + \Omega J, \qquad \Omega \in \mathfrak{so}(N). \end{aligned}$$

To solve the discrete Euler–Arnold equations (3):

- For $k = 0, 1, 2, \ldots$, find $\omega_k \in \mathrm{SO}(N)$ such that $M_k = \omega_k^\top J - J\omega_k$.
- Update $M_{k+1} = \omega_k M_k \omega_k^\top$.

By construction, this algorithm

- preserves exactly momentum and energy (integrable map)
- is a second order approximation to the continuous rigid body
- preserves the standard Poisson structure of $T^*\mathfrak{so}(N)$,

$$\{f, g\} = \mathrm{tr}(M[f_M, g_M]), \qquad f, g \in C^\infty(\mathfrak{so}(N)),$$

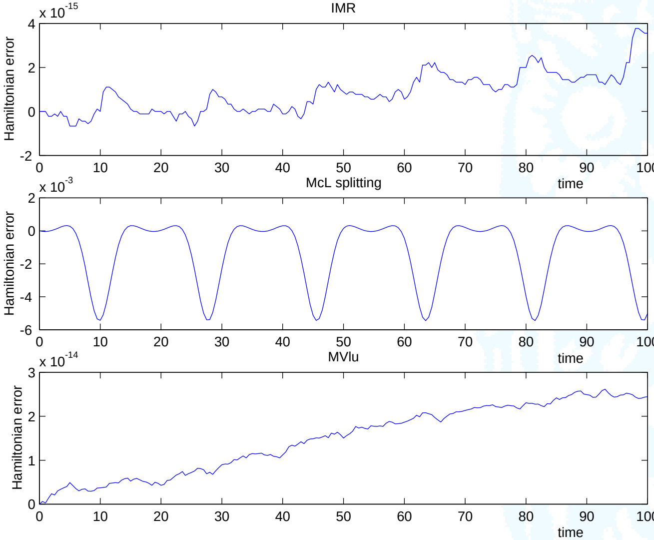
  where $f_M = (\partial f / \partial M_{i,j})$.

Note that

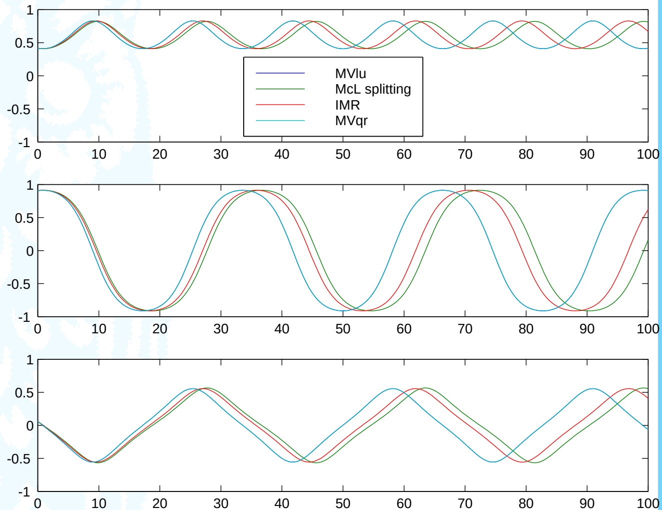
- Also the IMR is second order, preserves all the integrals of the continuous rigid body.
- Another much used method is a Lie–Poisson integrator of McLachlan and Reich (LP2). For the 3×3 RB, it consists in splitting the Hamiltonian

$$H = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_3 = \frac{m_1^2}{J_2 + J_3} + \frac{m_2^2}{J_1 + J_3} + \frac{m_3^2}{J_1 + J_2}$$

  and integrating explicitly (a la Strang) the vector fields of each split Hamiltonian. The method is second order, explicit, preserves the Poisson structure but does not preserve H.



Error in the Hamiltonian function H in the interval $[0, 100]$ and for $h = \frac{1}{2}$.



The components of the vector $\mathbf{m}_k$ for $h = \frac{1}{2}$...

$$\mathbf{m} = \begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix} \qquad \equiv \qquad \hat{\mathbf{m}} = M = \begin{bmatrix} 0 & -m_3 & m_2 \\ m_3 & 0 & -m_1 \\ -m_2 & m_1 & 0 \end{bmatrix}$$

Integrability of the Moser–Veselov equation

Recall the Moser–Veselov equation,

$$M_k = \omega_k^\top J - J\omega_k, \qquad M_k^\top = -M_k, \quad \omega_k^\top \omega_k = I. \tag{4}$$

in tandem with the update $M_{k+1} = \omega_k M_k \omega_k^\top$.

- The Moser–Veselov equation (4) has not a unique solution;

Lemma 1 *(Moser and Veselov) Equation* (4) *is equivalent to the factorization*

$$(I - \lambda M_k - \lambda^2 J^2) = (\omega_k^\top + \lambda J)(\omega_k - \lambda J)$$

Rewrite the above factorization as

$$(I - \lambda M_k - \lambda^2 J^2) = A_k^\top(\lambda) A_k(\lambda) \quad A_k(\lambda) = (\omega_k - \lambda J)$$

and define the mapping with image point M_{k+1} such that

$$(I - \lambda M_{k+1} - \lambda^2 J^2) = A_k(\lambda) A_k^\top(\lambda).$$

By construction,

$$(I - \lambda M_{k+1} - \lambda^2 J^2) = A_k(\lambda)(I - \lambda M_k - \lambda^2 J^2) A_k^{-1}(\lambda),$$

hence the map is an **integrable** as it is an isospectral flow.

BEA for DMV

Recall the DMV equations and the continuous RB equations

$$\begin{aligned} M_{k+1} &= \omega_k M_k \omega_k^\top, & M' &= [M, \Omega] \\ M_k &= \omega_k^\top J - J\omega_k, & M &= \Omega J + J\Omega, \end{aligned}$$

where $\omega_k \approx I - h\Omega(t_k)$.
We wish to write

$$M_{k+1} = \Phi_h(M_k) = M_k + h[M_k, \Omega_k] + h^2 d_2 + h^3 d_3 + h^4 d_4 + \cdots,$$

and find the modified vector field

$$\tilde{M}' = [\tilde{M}, \tilde{\Omega}] + h f_2(\tilde{M}, \tilde{\Omega}) + h^2 f_3(\tilde{M}, \tilde{\Omega}) + h^3 f_4(\tilde{M}, \tilde{\Omega}) + \cdots \tag{5}$$

such that $\Phi_h(M_k)$ equals the solution $\tilde{M}(t_{k+1})$ at time $t_{k+1} = t_0 + (k+1)h$ of the modified vector field (5).
To find $\Phi_k(h)$, we write

$$\omega_k = \exp(-h\Omega_0 - h^2\Omega_1 - h^3\Omega_2 - h^4\Omega_3 - h^5\Omega_4 + \cdots), \tag{6}$$

where $\Omega_0, \Omega_1, \Omega_2, \ldots,$ are skew-symmetric matrices computed so that

$$\omega_k^\top J - J\omega_k = h(\Omega(t_k)J + J\Omega(t_k)). \tag{7}$$

we obtain

$$h(\Omega(t_k)J + J\Omega(t_k)) = h(\Omega_0 J + J\Omega_0) + h^2(\Omega_1 J + J\Omega_1 + \tfrac{1}{2}(\Omega_0^2 J - J\Omega_0^2)) \\ + h^3(\Omega_2 J + J\Omega_2 + \tfrac{1}{2}[(\Omega_0\Omega_1 + \Omega_1\Omega_0), J] + \tfrac{1}{6}(\Omega_0^3 J + J\Omega_0^3)) + \cdots.$$

Comparing left and right-hand-sides, it is trivially observed that the order-h term disappears if $\Omega_0 = \Omega$ (to simplify notation, we omit the dependence of Ω on t_k). In order to annihilate the h^2-term, we require that

$$\Omega_1 J + J\Omega_1 + \frac{1}{2}(\Omega_0^2 J - J\Omega_0^2) = 0.$$

Recall that $M = \Omega J + J\Omega$ and hence $M' = \Omega' J + J\Omega'$. On the other hand, $M' = [M, \Omega] = -(\Omega^2 J - J\Omega^2)$. Hence we can write

$$O = \Omega_1 J + J\Omega_1 - \frac{1}{2}M' = \Omega_1 J + J\Omega_1 - \frac{1}{2}(\Omega' J + J\Omega')$$

and the identity is satisfied by if and only if

$$\Omega_1 = \frac{1}{2}\Omega'. \tag{8}$$

In general, the **algorithm** to derive Ω_i, for $i = 1, 2, \ldots$, is

1. Find the coefficient of h^{i+1} in (7) and set it equal to zero. This will give an equation of the type $\Omega_i J + J\Omega_i = C_i J + JC_i + [D_i, J]$. Note that the terms $C_i J + JC_i$ have an odd occurrence of the Ω_js, while the terms of the type $[D_i, J]$ have an even occurrence of the Ω_js.

2. Use the derivatives of M and Ω to express the term $[D_i, J]$ as $\tilde{C}_i J + J\tilde{C}_i$.

3. Deduce $\Omega_i = C_i + \tilde{C}_i$.

$$
\begin{array}{l}
\hline
\Omega_0 = \Omega \\
\Omega_1 = \frac{1}{2}\Omega' \\
\Omega_2 = \frac{1}{4}\Omega'' - \frac{1}{6}\Omega^3 \\
\Omega_3 = \frac{1}{8}\Omega''' - \frac{1}{24}(5\Omega^2\Omega' + 2\Omega\Omega'\Omega + 5\Omega'\Omega^2) \\
\hline
\end{array}
$$

The functions Ω_i

Once the Ω_is are known, substituting back in $M_{k+1} = \omega_k^\top M_k \omega_k$ and using the well known identity

$$\exp(X)Y\exp(-X) = \exp_{\mathrm{ad}_X} Y = \sum_{k=0}^{\infty} \frac{1}{k!}\mathrm{ad}_X^k(Y),$$

where $\mathrm{ad}_X(Y) = [X, Y]$ and, recursively, $\mathrm{ad}_X^k(Y) = [X, \mathrm{ad}_X^{k-1}(Y)]$, we find the expressions for the functions d_i in terms of the $\Omega_{i-1}, \Omega_{i-2}, \ldots, \Omega_0$,

$$d_i = \sum_{j=1}^{i} \frac{(-1)^j}{j!} \sum_{k_1+k_2+\cdots+k_j=i-j} \mathrm{ad}_{\Omega_{k_1}} \mathrm{ad}_{\Omega_{k_2}} \cdots \mathrm{ad}_{\Omega_{k_j}} M, \qquad k_1, \ldots k_j \in \{0, 1, \ldots, i-1\}. \tag{9}$$

$$
\begin{aligned}
d_2 &= \tfrac{1}{2}([M, \Omega'] + [[M, \Omega], \Omega]), \\
d_3 &= \tfrac{1}{4}[M, \Omega''] + \tfrac{1}{4}[[M, \Omega'], \Omega] + \tfrac{1}{4}[[M, \Omega], \Omega'] + \tfrac{1}{6}[[[M, \Omega], \Omega], \Omega] - \tfrac{1}{6}[M, \Omega^3], \\
d_4 &= \ldots,
\end{aligned} \tag{10}
$$

Taylor expansion of the solution of the modified equation

Consider

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{y} = f(\tilde{y}) + hf_2(\tilde{y}) + h^2 f_3(\tilde{y}) + \cdots,$$

where $f(M) = [M, \Omega] = [M, \mathcal{J}^{-1}M]$ is the original vector field of the RB equations, where $\mathcal{J}$ is a linear operator, defined such that $\mathcal{J}\Omega = \Omega J + J\Omega = M$. Putting $\tilde{y}(t) = M(t)$, we expand the solution of the above equation in a Taylor series and collect corresponding powers of h,

$$\begin{aligned}\tilde{y}(t+h) &= M(t) + hf(M) + h^2\left(f_2(M) + \frac{1}{2!}f'f(M)\right)\\ &\quad + h^3\left(f_3(M) + \frac{1}{2!}(f'f_2(M) + f_2'f(M)) + \frac{1}{3!}(f''(f,f)(M) + f'f'f(M))\right) + \cdots,\end{aligned}$$

where f' is considered as a linear operator, f'' as a bilinear operator and so on and so forth. In our case,

$$\begin{aligned}f'(z)(M) &= [z, \mathcal{J}^{-1}M] + [M, \mathcal{J}^{-1}z]\\ &= [z, \Omega] + [M, \mathcal{J}^{-1}z]\\ f''(z_1, z_2)(M) &= 2[z_1, \mathcal{J}^{-1}z_2],\end{aligned}$$

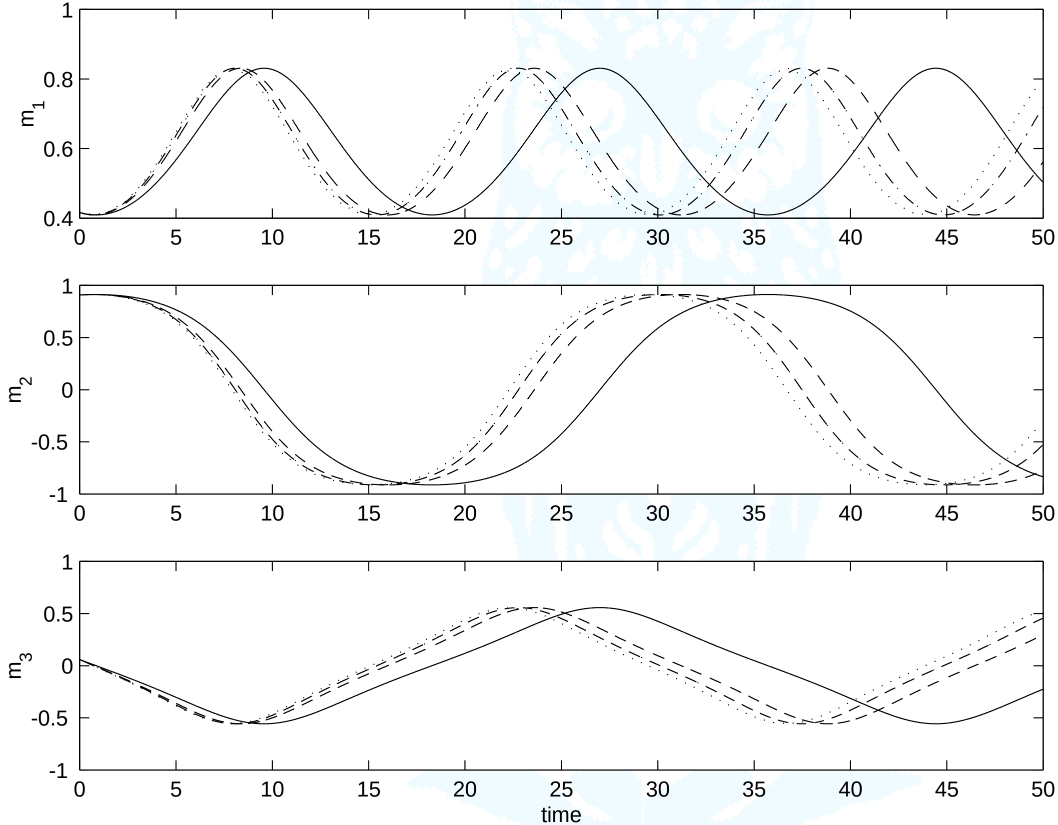
and, since f is quadratic, f''' and all the other higher derivatives equal zero.

At this point it is important to stress an important difference between the expressions for the modified vector field of (Hairer, Lubich & Wanner 2002) and ours. While the vector field discussed in (Hairer et al. 2002) is in $\mathbb{R}^n$, hence the f'' is a symmetric quadratic operator, this is not the case for our vector field which is on matrices, thus

$$f''(f'f, f) \neq f''(f, f'f).$$

This non-commutative case is discussed with more generality in (Munthe-Kaas & Krogstad 2002). However, we observe that *all* the terms containing combinations of f'', f' and f correspond simply to higher derivatives of f. The mixed terms are treated instead specifically.
After some algebra, we have

$$\begin{aligned}
f_2 &= d_2 - \tfrac{1}{2!} f' f(M) \\
&= O, \\
f_3 &= d_3 - \tfrac{1}{3!}(f''(f,f)(M) + f'f'f(M)) \\
&= \tfrac{1}{12}[M, \Omega'' - [\Omega, \Omega'] - 2\Omega^3], \\
f_4 &= d_4 - \tfrac{1}{4!} M^{(iv)} - \tfrac{1}{2!}(f' f_3 + f_3' f) \\
&= O, \\
f_5 &= d_5 - \tfrac{1}{5!} M^{(v)} - \tfrac{1}{2!}(f' f_4 + f_4 f' + \tfrac{1}{2!} \tfrac{\mathrm{d}}{\mathrm{d}t}(f_3' f + f' f_3)) \\
&= \tfrac{1}{80}[M, \Omega^{(iv)}] - \tfrac{1}{80}[M, [\Omega, \Omega''']] + \tfrac{3}{40}[M, \Omega^5 - \Omega'\Omega\Omega'] \\
&\qquad + \tfrac{1}{80}[M, [\Omega', \Omega'']] - \tfrac{1}{40}[M, \Omega\Omega''\Omega] - \tfrac{1}{20}[M, \Omega^2\Omega'' + \Omega''\Omega^2] \\
&\qquad + \tfrac{1}{20}[M, [\Omega^3, \Omega']] - \tfrac{1}{40}[M, \Omega'^2\Omega + \Omega\Omega'^2 + \Omega[\Omega, \Omega']\Omega].
\end{aligned} \tag{11}$$



The DMV solution of the RB equations (dotted line), the exact solution (solid line) and the trajectories corresponding to the modified vector fields $f + h^2 f_3$ (dashed line) and $f + h^2 f_3 + h^4 f_5$ (dash-dotted line) in the interval $[0, 50]$ with $h = \frac{8}{10}$.

Some important results about DMV

Theorem 2 *The DMV is time-reversible, hence* $f_{2i} = 0$*,* $i = 1, 2, \ldots$*.*

Theorem 3 *(Moser–Veselov) In the* 3×3 *case, the DMV is a time-reparamtetrisation of the flow of the original vector field of the rigid body.*

Since the mapping preserves the underlying Poisson structure and all the integrals $F_i = c_i$ of the system, it commutes with all commuting Hamiltonian flows generated by the F_is, $M' = \{M, \nabla F_i\}$. The nonsingular compact level sets $T_c = \cap_i(F_i = c_i)$ consists of a finite union of 1-dimensional tori and on each torus the DMV mapping is a shift along the trajectory depending on the integral quantity H_2.

Hence, the DMV solves the modified equation

$$M' = (1 + h^2\tau_3 + h^4\tau_5 + \cdots + h^{2i}\tau_{2i+1} + \cdots)[M, \Omega],$$

where h is the stepsize of integration and the τ_{2i+1}, for $i = 1, 2, \ldots$, are constants.

Introduce the constants

$$
\begin{aligned}
C_{J,i,j} &= J_1^i J_2^j + J_1^i J_3^j + J_2^i J_3^j, \\
C_{J,i} &= C_{J,i,i} \\
C_J &= C_{J,1} \\
\Delta &= (J_1 + J_2)(J_1 + J_3)(J_2 + J_3) \\
H_2 &= (J_1 + J_2)(J_1 + J_3)(J_2 + J_3)H - C_J \|\mathbf{m}\|_2.
\end{aligned}
$$

Theorem 4 *One has*

$$
\tau_3 = \frac{1}{6\Delta^2}((3\det(J)\mathrm{tr}(J) + C_{J,2})\|\mathbf{m}\|_2^2 + (3C_J + \mathrm{tr}(J^2))H_2),
$$

and

$$
\begin{aligned}
\tau_5 = \frac{1}{40\Delta^4}\Big(&(3\mathrm{tr}(J^4) + 27C_{J,2} + 15\mathrm{tr}(J^2)C_J + 45\det(J)\mathrm{tr}(J))H_2^2 \\
&+ (10C_{J,3} + 50\det(J)\mathrm{tr}(J)C_J + 10\det(J)\mathrm{tr}(J)\mathrm{tr}(J^2) + 2C_{J,2}\mathrm{tr}(J^2) - 28\det(J^2))\|\mathbf{m}\|_2^2 H_2 \\
&+ (60\det(J^2)C_J + 3C_{J,4} + 27\det(J^2)\mathrm{tr}(J^2) + 15\det(J)(C_{J,2,3} + C_{J,3,2}))\|\mathbf{m}\|_2^4\Big).
\end{aligned}
$$

Proof. By direct computation of f_3 and f_5. □

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Higher-order integrable methods

For the original RB equations, scaling the initial condition is equivalent to scaling time.
In our case, we know that DMV is a time-rescaling of the original RB equation. Therefore we wish to rescale the initial condition to obtain a better approximation of the unscaled original RB.

I.C. DMV	New I.C. DMV
$h(\Omega(t_k)J + J\Omega(t_k))$	$\frac{h(\Omega(t_k)J+J\Omega(t_k))}{1+\tilde{\tau}_3h^2+\tilde{\tau}_5h^4+\cdots}$

We perform again the backward error analysis. We set now $\tilde{\omega} = \exp(-h\tilde{\Omega}_0 - h^2\tilde{\Omega}_1 + \cdots)$ and solve for the $\tilde{\Omega}_i$s as the skew-symmetric matrices that solve

$$h(1 - \tilde{\tau}_3 h^2 + (\tilde{\tau}_3^2 - \tilde{\tau}_5)h^4 + \cdots)(\Omega J + J\Omega) = \tilde{\omega}^\top J - J\tilde{\omega}. \tag{12}$$

$$\begin{aligned} \tilde{f}_3 &= \tilde{d}_3 - \frac{1}{3!}M''' = -\tilde{\tau}_3[M,\Omega] + d_3 - \frac{1}{3!}M''' \\ &= -\tilde{\tau}_3[M,\Omega] + f_3 = (-\tilde{\tau}_3 + \tau_3)[M,\Omega], \end{aligned}$$

hence, in order to have an order-four scheme, we must set $\tilde{f}_3 = 0$ which corresponds to the choice

$$\tilde{\tau}_3 = \tau_3.$$

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After further computations, one has

$$\tilde{f}_5 = 0 \leftrightarrow \tilde{\tau}_5 = \tau_5 - 2\tau_3^2.$$

This value of $\tilde{\tau}_5$ gives indeed a method of order six.
The new proposed algorithms of order four and six are described below.

The DMV4 algorithm:

1. Compute τ_3 and set $M_0 := M(t_0)h/(1 + h^2\tau_3)$.
2. For $k = 0, 1, \ldots, n-1$,
   find the unique w_k as above such that $M_k = \omega_k^\top J - J\omega_k$
   set $M_{k+1} = \omega_k M_k \omega_k^\top$
   end
3. Reconstruct $M_n := M_n(1 + h^2\tau_3)/h \approx M(t_n)$.

The DMV6 algorithm:

1. Compute τ_3, τ_5 and set $\tilde{\tau}_5 = \tau_5 - 2\tau_3^2$ and $M_0 := M(t_0)h/(1 + h^2\tau_3 + h^4\tilde{\tau}_5)$.
2. For $k = 0, 1, \ldots, n-1$,
   find the unique w_k as above such that $M_k = \omega_k^\top J - J\omega_k$
   set $M_{k+1} = \omega_k M_k \omega_k^\top$
   end
3. Reconstruct $M_n := M_n(1 + h^2\tau_3 + h^4\tilde{\tau}_5)/h \approx M(t_n)$.

Some numerical experiments

We consider with initial condition

$$\mathbf{m}_0 = \begin{bmatrix} 0.4165 \\ 0.9072 \\ 0.0588 \end{bmatrix}$$

and matrix J given as

$$J = \begin{bmatrix} 0.9218 & 0 & 0 \\ 0 & 0.7382 & 0 \\ 0 & 0 & 0.1763 \end{bmatrix}$$

and compare the DMV explicit scheme with the Hamiltonian-splitting method LP2 of (McLachlan 1993)

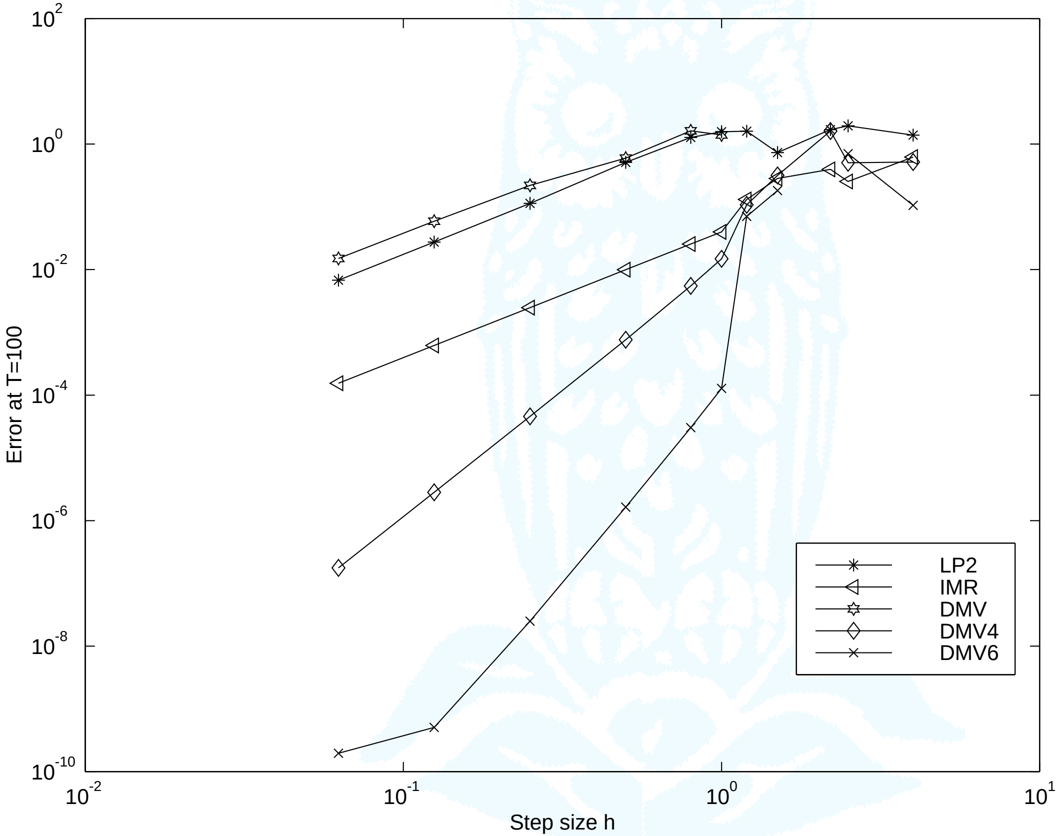
$$H = \frac{m_1^2}{J_2 + J_3} + \frac{m_2^2}{J_1 + J_3} + \frac{m_3^2}{J_1 + J_2} = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_3$$

and the Implicit Midpoint Rule (IMR),

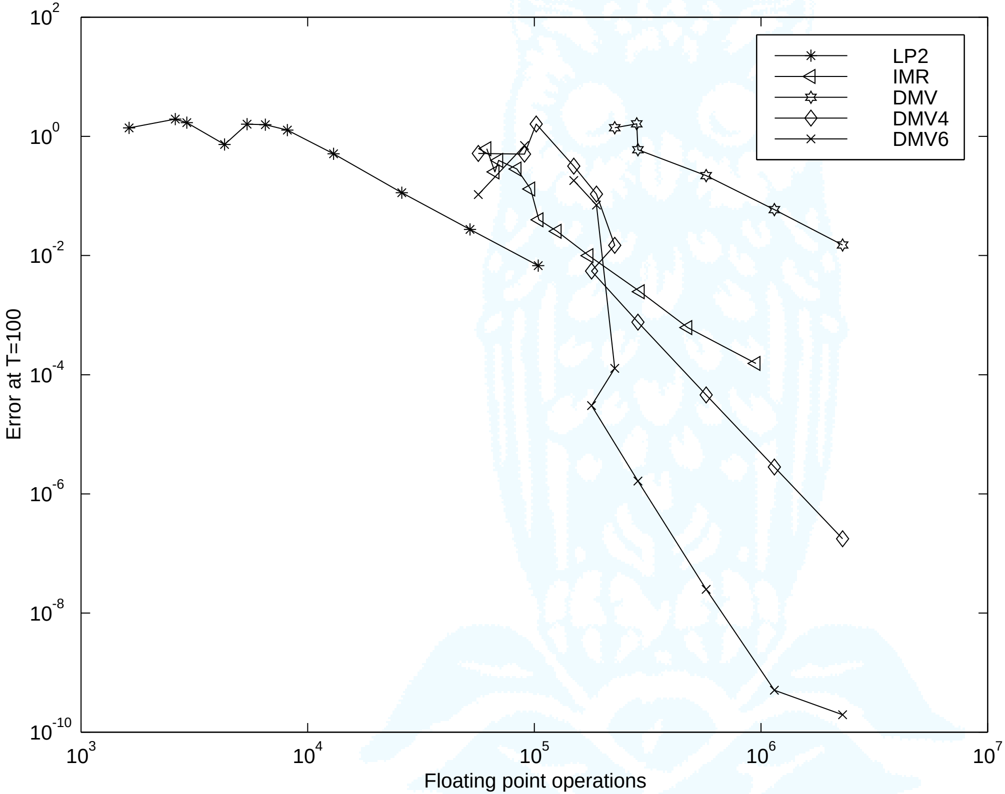
$$\mathbf{m}_{k+1} = \mathbf{m}_k + h\mathbf{f}(\frac{\mathbf{m}_k + \mathbf{m}_{k+1}}{2}),$$

where

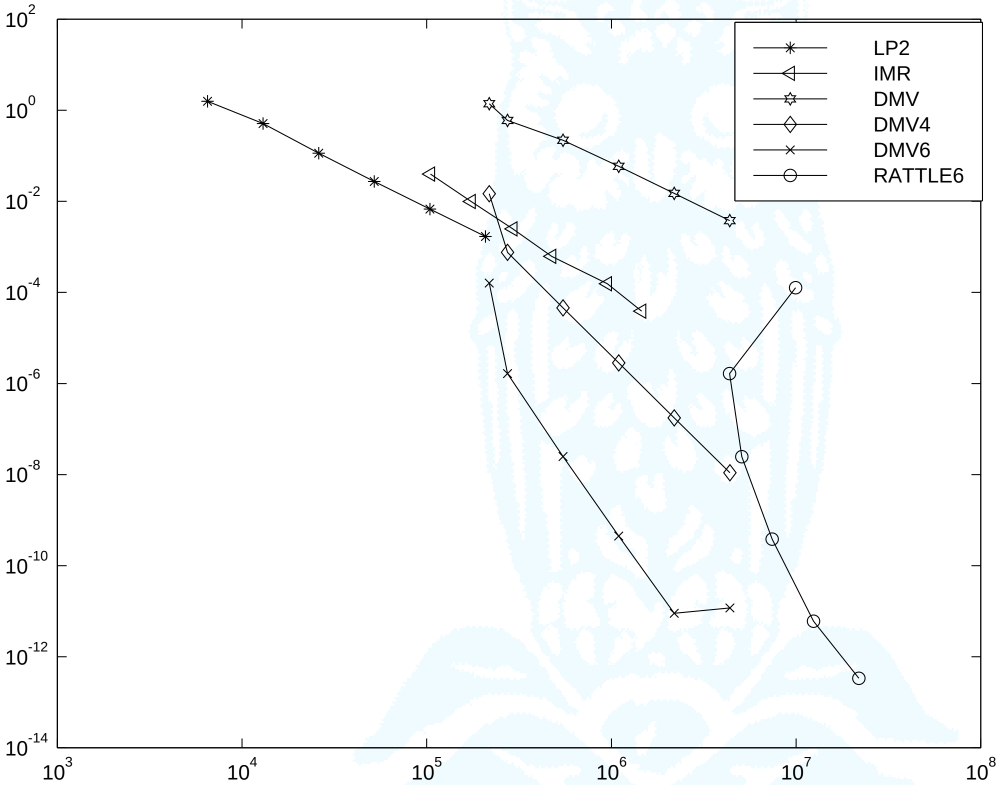
$$\mathbf{f}(\mathbf{m}) = \mathbf{m} \times (\tilde{J})^{-1}\mathbf{m}, \qquad \tilde{J} = \begin{bmatrix} J_2 + J_3 & 0 & 0 \\ 0 & J_1 + J_3 & 0 \\ 0 & 0 & J_1 + J_2 \end{bmatrix}.$$



Error versus step size computed at $T = 100$ for the methods LP2, IMR, DMV, DMV4, DMV6.



Floating point operations versus accuracy ($T = 100$) for the methods LP2, IMR, DMV, DMV4, DMV6. The roots of $P(\lambda)$ are recomputed at each step, use QR with pivoting, (DMV ≈ 22 LP2 per step).



Floating point operations versus accuracy ($T = 100$) for the methods LP2, IMR, DMV, DMV4, DMV6 and RATTLE6. The roots of $P(\lambda)$ are computed once, use LU instead of QR (DMV ≈ 19

LP2 per step).

Method	$h = \frac{1}{16}$	$h = \frac{1}{2}$	$h = 1.2$	$h = 2.2$	$h = 2.5$	$h = 4$
LP2	6.7903e-03	5.1043e-01	1.6055e+00	1.7002e+00	1.9489e+00	1.3902e+00
IMR	1.5494e-04	9.9329e-03	1.3119e-01	3.9514e-01	2.5276e-01	6.1905e-01
DMV	1.5014e-02	5.9899e-01	NaN	NaN	NaN	NaN
DMV4	1.757e-07	7.6167e-04	1.0785e-01	1.6094e+00	5.0245e-01	5.1624e-01
DMV6	1.962e-10	1.6440e-06	7.0269e-02	NaN	7.0407e-01	1.0519e-01

Error for the various methods and selected step sizes

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Connections with matrix Ricatti equations

Consider the matrix equation

$$M = XJ - JX^\top. \tag{13}$$

Cardoso & Leite (2003) shown that every solution of (13) (not necessarily orthogonal) is of the form

$$X = (M/2 + S)J^{-1},$$

for some symmetric matrix S.
Furthermore, X is a *orthogonal* solution of (13) if and only if S is a symmetric solution of the Riccati equation

$$S^2 + S(M/2) + (M/2)^\top S - (M^2/4 + J^2) = 0. \tag{14}$$

Riccati equations are associated to symplectic matrices. In our case, the symplectic matrix is

$$H_{\mathrm{sympl}} = \begin{bmatrix} \frac{M}{2} & I \\ \frac{M^2}{4} + J^2 & \frac{M}{2} \end{bmatrix}. \tag{15}$$

If $\frac{M^2}{4} + J^2$ is positive definite, it has been shown in (Cardoso & Leite 2003) that (14) has a unique solution S which is symmetric, positive definite, and such that the eigenvalues of $W = M/2 + S$ have positive real parts. This matrix W is precisely the same matrix in Moser & Veselov (1991), from which one obtains

$$\omega = WJ^{-1}.$$

Algorithm(Cardoso & Leite 2003): Compute X, the unique solution of (13) in the special orthogonal group $\mathrm{SO}(n)$.

1. Find a real Schur form of H_{sympl},

$$\tilde{Q}^\top H_{\text{sympl}} \tilde{Q} = \begin{bmatrix} T_{11} & T_{12} \\ O & T_{22} \end{bmatrix}, \tag{16}$$

   where T_{11} and T_{22} are block upper-triangular matrices such that the real parts of the spectrum of T_{11} are positive and the real parts of the spectrum of T_{22} are negative definite.

2. Partition $\tilde{Q}$ accordingly,

$$\tilde{Q} = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix}.$$

   Then, compute

$$S = Q_{21} Q_{11}^{-1}.$$

3. Compute

$$X = \left(\frac{M}{2} + S \right) J^{-1}.$$

Some computational details

- Compute real Schur forms by QR iterations for eigenvalues (Golub & van Loan 1989)
- Cost: $\mathcal{O}((2N)^3)$ operations (implicit methods for ODEs: $\mathcal{O}(N^3)$)

N being the dimension of M.

The case $N = 3$

In this case,

- it is possible to find an **explicit spectral decomposition** of H_{sympl} (without the QR eigenvalue method)
- construct the real Schur decomposition (16) and hence X from the eigenstructure of H_{sympl}.

This yields an **explicit** numerical method for the reduced RB equations.

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The eigenvalues of the matrix H_{sympl},

$$H_{\text{sympl}} = \begin{bmatrix} \frac{M}{2} & I \\ \frac{M^2}{4} + J^2 & \frac{M}{2} \end{bmatrix} \tag{17}$$

are the solutions of the **quadratic eigenvalue problem**

$$P(\lambda) = \det(\lambda^2 I - \lambda M - J^2) = 0.$$

Without loss of generality, we assume that J is diagonal, with entries J_1, J_2, J_3. Then,

$$\begin{aligned} -P(\lambda) &= \lambda^6 - \lambda^4 \left(J_1^2 + J_2^2 + J_3^2 - m_{12}^2 - m_{13}^2 - m_{23}^2\right) \\ &\quad + \lambda^2 \left(J_1^2 J_2^2 + J_1^2 J_3^2 + J_2^2 J_3^2 - m_{12}^2 J_3^2 - m_{13}^2 J_2^2 - m_{23}^2 J_1^2\right) - J_1^2 J_2^2 J_3^2 \\ &= \lambda^6 - \lambda^4(\operatorname{tr}(J^2) - \|\mathbf{m}\|_2) + \lambda^2(C_{J,2} - H_2) - \det(J^2). \end{aligned} \tag{18}$$

$$\begin{aligned} C_{J,i,j} &= J_1^i J_2^j + J_1^i J_3^j + J_2^i J_3^j, \\ C_{J,i} &= C_{J,i,i} \\ C_J &= C_{J,1} \\ H_2 &= (J_1 + J_2)(J_1 + J_3)(J_2 + J_3)H - C_J\|\mathbf{m}\|_2. \end{aligned}$$

- Reduce to a cubic equation (compute the roots explicitely)

Schematical procedure

- Compute eigenvalues/eigenvectors of H_{sympl}:

$$H_{\text{sympl}} \begin{bmatrix} Y_1 & Y_2 \end{bmatrix} = \begin{bmatrix} Y_1 & Y_2 \end{bmatrix} \begin{bmatrix} \Lambda_+ & \\ & \Lambda_- \end{bmatrix}, \qquad \operatorname{Re} \Lambda_+ \geq 0,$$

(the eigenvectors need not be orthogonal and may be complex). $Y_1, Y_2 \in \mathbb{R}^{6\times 3}, \Lambda_\pm \in \mathbb{R}^{3\times 3}$.

- Orthogonalize the eigenvectors (by Grahm-Schmidt or QR),

$$[Y_1, Y_2] = QR,$$

so that

$$H_{\text{sympl}} Q = QR\Lambda R^{-1}$$

is the complex Schur form.

- Reduce to a real Schur form by considering real/imaginary part (complex Givens rotation).
- Compute $\quad S = Q_{21} Q_{11}^{-1}, \quad X = (M/2 + S) J^{-1}$.

- We don't need all the eigenvectors, just Y_1. Don't need R.
- Avoid complex arithmetic alltogether.

The numerical DMV algorithm

- $\mathbf{m}_0 \mapsto hM_0 = h\hat{\mathbf{m}}_0$.
- Compute the eigenvalues of $H_{\mathrm{sympl}} = H(M_k)$ solving for $P(\lambda) = 0$ as in (18).
- For $t_k = t_0 + kh$, $k = 0, 1, 2 \ldots$
  - Compute the (real) eigenvectors corresponding to Λ_+
    - Compute 3 'quadratic' eigenvectors (3 matrix factorizations, LU/QR, with pivoting). No need to compute explicitely L or Q.
    - Compute the 'dependent' eigenvectors.
  - Orthogonalize the eigenspace
    - By (modified) Grahm–Schmidt or QR. Only the Q factor is needed.
  - Compute $\quad S = Q_{21}Q_{11}^{-1}, \quad \omega_k = (M/2 + S)J^{-1}$
    - Update $M_{k+1} = \omega_k^\top M_k \omega_k$
- Rescale $\mathbf{m}_N \leftarrow M_N/h$.

This algorithm produces an explicit method that is about $20 - 22$ times more expensive than LP2, the explicit method of McLachlan and Reich.

Concluding remarks

- **Explicit** algorithms to solve for the $N = 3$ free rigid body
- The methods are up to 6th order, completely integrable, possible to increase to arbitrary order
- The cost of the method is about $10 - 22$ times more expensive than the explicit LP2. The cheaper versions seem to be less stable expecially for large step-size and long time computations
- Reconstruction equations: Find the configuration

  $$X_{k+1} = X_k \omega_k^\top .$$

  The complexive order is still 2 but the error is generally smaller. Backward error analysis reveals that some error terms cancel, however the components are reparametrized with 3 different time scales.

  To obtain higher order reconstructions, one can use interpolation of the vector field $X\Omega$ and its higher derivatives using the computed values of Ω_k.
- Optimal step-size?

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